

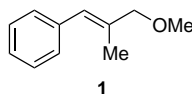
## Additions and Corrections

### Asymmetric Hydrogenation of Unfunctionalized Trisubstituted Olefins with a Chiral Titanocene Catalyst

[*J. Am. Chem. Soc.* **1993**, *115*, 12569–12570].

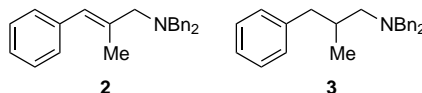
RICHARD D. BROENE AND STEPHEN L. BUCHWALD\*

Page 12569: The compound shown in ref 13 is incorrect. The correct structure is **1**, shown below, and is therefore incapable of the  $\beta$ -alkoxide elimination reaction suggested in ref 13.



Page 12570: The starting material and products for entry 8 of Table 1 should be compounds **2** and **3**, respectively. This error does not alter the percent ee observed for this entry or the conclusions of the paper.

JA965416K



S0002-7863(96)05416-9

## Book Reviews \*

**Electronic Structure Calculations on Fullerenes and Their Derivatives.** By Jerzy Cioslowski (Florida State University). Oxford University Press: New York. 1995. ix + 281 pp. \$65.00. ISBN 0-19-508806-9.

The rapid growth of fullerene research has generated an enormous literature on quantum chemical computations of the electronic structure and properties of these interesting molecules. In this text, the author provides a current account of this large body of work from a theoretical chemist's viewpoint. In order that the book be self-contained, it includes a chapter reviewing quantum chemical approaches to the calculation of electronic structure that serves as a useful reference for the applications and results in subsequent chapters. The book's subject material spans the full breadth of fullerene research, with chapters organized around individual classes of fullerenes, fullerene derivatives, and materials. Although the text is chiefly concerned with theoretical treatments of fullerenes, each chapter contains an introduction that briefly describes the current state of relevant experimental measurements. Most researchers studying fullerenes will find at least one chapter devoted to their particular research focus.

$C_{60}$  and  $C_{70}$ , the most abundantly produced and widely studied fullerenes, are treated in separate chapters, each with extensive tables comparing the results of different theoretical methods for the calculation of bond lengths, vibrational frequencies, orbital energies, excited state energies, heat of formation, ionization potential, electron affinity, and polarizability. The theoretical methods employed range from the semiempirical to *ab initio* calculations. Together, these two chapters include nearly 400 references to the literature.

Other chapters are devoted to medium-sized fullerenes, large carbon clusters, small fullerenes, endohedral complexes, heterofullerenes, fullerene derivatives, and solid-state fullerenes. The discussion of "medium size" fullerenes includes computations on  $C_{76}$ ,  $C_{78}$ ,  $C_{82}$ , and  $C_{84}$ . These species have more complicated, lower-symmetry structures than  $C_{60}$  or  $C_{70}$ , and each has many possible geometric isomers. Tables are included, giving the relative heats of formation of the isolated pentagon isomers calculated by more than a dozen different quantum chemical methods. The chapter covering the large spheroidal and tubular fullerenes, graphitic microtubules, and hypothetical polymeric

allotropes of carbon is brief, but offers extensive references to more detailed accounts in the literature.

Fullerene metal endohedral complexes are discussed in considerable detail. Perturbation theory is shown to be useful for the calculation of the electronic structures of endohedral complexes because mixing between the orbitals of the host and the guest is expected to be negligible. Some interesting results of these calculations are given.

This book offers an extensive review of the current state of theoretical studies of the fullerenes. It provides a bridge between the quantum chemistry textbook and the research literature describing detailed applications of quantum chemical methods applied to fullerenes. Because of the great breadth of coverage and abundant up-to-date references, this book will be a valuable addition to the libraries of both experimentalists and theoreticians interested in fullerenes.

Anthony H. Francis, *The University of Michigan*

JA9553157

S0002-7863(95)05315-7

**Studies in Surface Science and Catalysis-91: Preparation of Catalysts VI: Scientific Bases for the Preparation of Heterogeneous Catalysts.** Edited by G. Poncelet (Universite Catholique de Louvain, Belgium), J. Martens (Katholieke Universiteit, Belgium), B. Delmon (Universite Catholique de Louvain, Belgium), P. A. Jacobs (Katholieke Universiteit, Belgium), and P. Grange (Universite Catholique de Louvain, Belgium). Elsevier: Amsterdam. 1995. xxi + 1182 pp. \$350.00. ISBN 0-444-82078-7.

This book is based on the proceedings of the Sixth International Symposium, held in Louvain-La-Neuve, Belgium, September 5–8, 1994. The organizers of this symposium maintained their initial objectives to gather experts from both industries and universities to discuss the scientific problems involved in the preparation of heterogeneous catalysts, and to encourage as much as possible the presentation of research work on catalysts of real industrial significance. Another highlight of these symposia is to reserve a substantial part of the program for new developments in catalyst preparation, new preparation methods, and new catalytic systems. The fact that chemical reactions

\*Unsigned book reviews are by the Book Review Editor.

which were hardly conceivable some years ago have become possible today through the development of appropriate catalytic systems proves that catalysis is in constant progress. The papers in this volume deal with preparation of new catalysts and supports, catalyst preparation via sol-gel methods, supported catalysts, and synthesis of nanometer-size catalysts.

JA9656210

S0002-7863(96)05621-1

**Halon Replacements: Technology and Science.** Edited by Andrzej W. Miziolek (U.S. Army Research Laboratory) and Wing Tsang (National Institute of Standards and Technology). ACS: Washington, DC. 1995. xi + 388 pp. \$99.95. ISBN 0-8412-3327-6.

ACS Symposium Series 611. Developed from a symposium sponsored by the Division of Environmental Chemistry, Inc., at the 208th National Meeting of the American Chemical Society, Washington, DC, August 21–25, 1994. This volume presents a comprehensive and up-to-date examination of research, development, and testing for Halon replacements. The current scientific basis for government regulatory decisions mandating Halon phaseout is discussed. The related environmental issues, including atmospheric chemistry and modeling, corrosivity, and toxicology, are addressed. The progress in understanding the chemistry of flame inhibition as well as state-of-the-art databases for computer simulation of this complex chemistry is reported.

JA9655956

S0002-7863(96)05595-3

**Thermochemical Data of Pure Substances Third Edition, Two Volumes, Vol. 1: Ag-Kr and Vol. II: La-Zr.** By Ihsan Barin (ZEUS GmbH, FRG), in collaboration with Gregor Platzki. VCH: New York. 1995. 1900 pp. \$535.00. ISBN 3-527-28745-0.

This is the revised, extended, up-to-date third edition of the reference book *Thermochemical Data of Pure Substances*. This two-volume set covers 3300 pure substances, and also includes 230 organic compounds, all of which are tabulated. This book discusses subjects ranging from heat capacity, entropy, and Gibbs energy function to enthalpy of formation, equilibrium constant of formation, and the thermodynamics of the processing of ores, coal, waste, and residues. The introductory section discusses thermodynamic theory and applications concisely and explains how best to use the tables.

JA965624C

S0002-7863(96)05624-7

**Advances in Theoretically Interesting Molecules, Vol. 3.** Edited by Randolph P. Thummel (University of Houston). JAI: Greenwich. 1995. x + 316 pp. \$97.50. ISBN 1-55938-698-3.

This book maintains the same successful format that characterized the first two volumes in the series (1989 and 1992), with six chapters on six unrelated classes of theoretically interesting molecules written by prominent contributors to each of the areas covered. Several of the chapters include significant amounts of previously unpublished data from the authors' own research.

The first chapter, Polynuclear Aromatic Hydrocarbons with Curved Surfaces: Hydrocarbons Possessing Carbon Frameworks Related to Buckminsterfullerene, by P. W. Rabideau and A. Sygula, recounts briefly the birth of this field in 1966 with Lawton's synthesis of corannulene and then focuses on the rapid development of the field since its rebirth in 1991 with the introduction of a new high-temperature gas phase ring closure strategy for constructing such strained ring systems. Syntheses and properties of fullerene subunits up to C<sub>30</sub>H<sub>12</sub> are described and are nicely augmented by extensive theoretical calculations. Interest in this important field has paralleled the intense research on C<sub>60</sub> and the higher fullerenes over the last five years.

The two chapters Chemistry of Cyclopropanes, by P. Müller, and Radical Cations of Cyclopropane Systems: Conjugation and Homoconjugation with Alkene Functions, by H. Roth, constitute very scholarly and well-balanced overviews of more mature families of theoretically interesting molecules: mostly isolable compounds in the former case and novel reactive intermediates in the latter. About these

two families, much is already known, yet both represent areas of continuing research activity, as evidenced by the large number of recent literature citations, many from the authors' own laboratories.

The chapter provocatively entitled Mills-Nixon Effects? by N. L. Frank and J. S. Siegel endeavors first to squeeze the last breaths out of the obsolete but still lingering concept known to chemists as the Mills-Nixon effect and then turns to address the very real questions of how various structural features in annulated benzenoid compounds can influence (1) deviations from bond convergence in the aromatic ring and (2)  $\alpha/\beta$  reactivity ratios. An exceptionally thorough and systematic analysis of data collected from every conceivable vantage point and reproduced in 14 pages of tables and graphs makes a convincing case that these authors have succeeded in identifying what is important and what is irrelevant in this heretofore confusing quagmire.

Henry Wong's chapter Planar Dehydro[8]annulenes and Other Theoretically Interesting Molecules presents a very personal account of the author's own research career, which I happened to enjoy reading, but it is more a pleasant stroll down memory lane, from 8-membered ring hydrocarbons to 5-membered ring heterocycles, than a critical summary of a single subject.

The chapter Infrared Spectroscopy of Highly Reactive Organic Species: The Identification of Unstable Molecules and Reactive Intermediates Using *ab Initio* Calculated Infrared Spectra, by B. A. Hess and L. Smentek, provides a wonderful picture of the early developments in this field and leaves one impressed with the power of modern computational methods not only to reproduce the IR spectra of matrix-isolated reactive species but to provide reliable predictions of IR spectra that can help guide experimentalists in their search for new species. Regrettably, this chapter draws examples primarily from the older literature, with only a handful of references in the 1990s.

The short tables of contents at the beginning of each chapter and the composite 12-page subject index at the end of the book all facilitate quick access to specific topics; however, the author index is disgracefully incomplete. Nearly 1000 references to the chemical literature are cited in the six chapters, and most of those have two or more authors, yet the author index lists only 126 names and even fails to mention five of the authors and coauthors of these chapters. Apparently, JAI Press and the editor have compiled this index solely from those citations for which the names of one or more authors happened to be mentioned explicitly in the text of a chapter. Notwithstanding this one shortcoming, the book pulls together huge amounts of scattered information and organizes it in a manner that will prove valuable to experts in the field and informative to the newcomers.

Lawrence T. Scott, Boston College

JA955355A

S0002-7863(95)05355-8

**Cytochrome *c*—A Multidisciplinary Approach.** Edited by R. A. Scott (University of Georgia) and A. G. Mauk (University of British Columbia). University Science Books: Sausalito, CA. 1996. vi + 738 pp. \$85.00. ISBN 0-935702-33-4.

In 1987 and 1990 G. R. Moore and G. W. Pettigrew coauthored two volumes on the cytochromes *c* which have become standard reference works in the field. How does the present multiauthored volume compare? Like most multiauthor books it suffers from some unevenness of approach. However, all the contributors are authorities in their areas, and most of the reference lists bring Moore and Pettigrew up to date.

There are some quite general and other rather specialized articles. The opening chapter by Emanuel Margoliash is an important summary of the history of the field seen through the eyes of the man who was responsible for initiating the bulk of modern work on cytochrome *c* structure and evolution. The evolutionary chapter which follows (T. E. Meyer) prides itself on using no extensive "tree" diagrams (indeed is free from diagrams except for one very schematic version). It does indeed broaden the picture with the numerous prokaryotic cytochromes *c* now known, but the reviewer regrets having to go back to Dickerson's 1980 *Scientific American* article to get a global picture of the eukaryotic and prokaryotic proteins and their relationships. Indeed the absence of color plates or even halftone pictures from the volume may have been a cost saver but detracts from a modern presentation of a topic like this. Even Brayer and Murphy's extensive and detailed article on structure does not go beyond some rather simplified stereo diagrams and some poorly reproduced ball and stick figures evidently copied

from colored originals. This is a pity considering the importance of the recent work summarized in this chapter. Pielak *et al.* and Hildebrandt effectively summarize current ideas on NMR and resonance Raman spectroscopy of these cytochromes, but the volume lacks chapters (in its "spectroscopy" section) not only on the important magnetic methods EPR and MCD but even on UV-vis spectroscopy, by means of which these proteins were originally discovered and which would have given the opportunity to include definitive spectra of the different *c* cytochromes and their derivatives.

Other important topics not covered in this work include all the genetic and molecular biological information on cytochromes *c*, or any mention of gene expression and biosynthesis, or tissue specificity (e.g., the remarkable testicular form) or isozymes (e.g., the two yeast iso forms). Ligand reactions of the protein are considered only in its proteolytically modified and misnamed "microperoxidase" forms (a useful chapter by the South African group of Adams *et al.*) and the alkaline transition, effectively summarized by Wilson and Greenwood.

There is a strong emphasis on the chemistry of the protein which may add to the volume's appeal to *Journal of the American Chemical Society* readers, with separate chapters on electrochemistry (Hill *et al.*), chemical modification (Millett and Durham), metal complex cross-linking (Kostic), and semisynthesis (Wallace). Functional (physiological electron transfer) activity is less satisfactorily treated and divided between different rather brief articles by Millett and by Cusanovich and Tollin. Biophysics of electron transfer and protein-protein interactions are covered by Scott and Northrup with the thermodynamics treated by Schejter. The more biological aspects of cytochrome *c*-enzyme and -membrane interactions are split between chapters on electrostatics (Gunner and Honig), protection methodology (Bosshard), and apo- and holo-protein comparisons (Jordi and De Kruijff) as well as some of the chapters mentioned above. This does not allow a good overview of the problems involved in cytochrome *c* binding which remains a problematic area even though we have crystal structures not only for the small soluble cytochrome *c* peroxidase protein but also for two cytochrome *c* oxidases.

In summary, (i) the most important omission—molecular biology (this may be a plus in some eyes), (ii) the most significant drawback—a lack of good illustrations, and (iii) the most valuable aspect—significant coverage of cytochrome *c* chemistry by well-respected authorities. Overall verdict: it will not replace the two volumes by Moore and Pettigrew but provides an important update at a reasonable price by current standards and therefore a book which should be in all cytochrome *c* chemists' libraries (or those of their institutions).

References: Pettigrew, G. W.; Moore, G. R. *Cytochromes c: Biological Aspects*; Springer-Verlag: New York, 1987. Moore, G. R.; Pettigrew, G. W. *Cytochromes c: Evolutionary, Structural and Physicochemical Aspects*; Springer-Verlag: New York, 1990.

Peter Nicholls, Brock University, Canada

JA9655911

S0002-7863(96)05591-6

**Photographic Sensitivity: Theory and Mechanisms.** By Tadaaki Tani (Fuji Photo Film Co.). Oxford University Press: New York and Oxford. 1995. viii + 254 pp. \$75.00. ISBN 0-19-507240-5.

Many years have passed since the publication of texts on the physical chemical aspects of photography, and even the most recent of those were highly derivative of the 4th edition of *The Theory of the Photographic Process*, edited by T. H. James and published in 1977. Now Tadaaki Tani fills this need with a brief, but up-to-date and authoritative book. It appears that English is not Tani's native language, but his writing is clear, and one has little difficulty understanding the discussions of even complicated matters. The older literature is fairly represented, but recent citations favor work of the Fuji Photo Film Co., where the author has spent three decades studying photographic sensitivity.

Photographic phenomena are discussed and interpreted from a molecular or "microscopic" point of view, invoking modern concepts of grain crystal structure, solid state behavior, surface science, and electron transfer. Practical and technological aspects of photography are seldom discussed.

In the first part of the book, the properties of silver halide photographic materials are discussed, with comparison, when appropriate, to electronic photography. Then the mechanism of latent image formation is discussed. Next, sensitization (broken down into spectral

sensitization by adsorbed dyes, so-called chemical sensitization, hypersensitization, and latensification) is covered. These topics are followed by discussion of theories of development—amplification of the latent image.

Tani makes it clear that he believes that silver halide photography is not yet dead, and he shows where improvements can be made in emulsion preparation and in photographic processing. Obviously this book will aid the scientists who hope to make these improvements.

William L. Jolly, University of California, Berkeley

JA965638I

S0002-7863(96)05638-7

**Progress in Clinical and Biological Research, Volume 394. Cellular and Molecular Mechanisms of Hormonal Carcinogenesis: Environmental Influences.** Edited by James Huff (National Institute of Environmental Health Sciences), Jeff Boyd (University of Pennsylvania Medical Center), and J. Carl Barrett (National Institute of Environmental Health Sciences). Wiley-Liss: New York. 1996. xiii + 480 pp. \$139.00. ISBN 0-471-02202-0.

The influence of hormonal perturbations on carcinogenesis is attracting increased research attention, a trend encouraged by the growing number of both natural and synthetic hormone-mimetic agents found in certain drugs, industrial products or wastes, and elsewhere in the environment. This book offers an authoritative, up-to-date overview of the role of environmental factors in the development of hormonally modulated cancers, as well as a comprehensive account of the latest research into the basic mechanisms of hormonal carcinogenesis in both human and animal models. Some of the topics covered are Dietary influences on carcinogenesis, Transplacental hormonal carcinogenesis, Estrogen as a carcinogen: genetics and molecular biology of human endometrial carcinoma, Mechanisms of chemically induced follicular cell carcinogenesis of the thyroid gland, and Environmental causes of breast cancer: future research directions.

JA9656098

S0002-7863(96)05609-0

**Electronic Materials Chemistry: An Introduction to Device Processes and Material Systems.** Edited by H. Bernhard Pogge (IBM Corp.). Dekker: Monticello, NY. 1996. xiii + 623 pp. \$195.00. ISBN 0-8247-9632-2.

The 13 chapters of this book successfully introduce the upper division undergraduate and graduate chemistry student to a wide-ranging set of topics dealing with the chemistry involved in electronic materials and electronic materials processing. Written by a crew of 13 chapter authors, with an editor at the helm, the chapters provide a pleasant and easy-to-read introduction that, true to the title, stress chemical issues.

The first chapter is an excellent primer on electronic products and sets the stage for what follows—six chapters on processes and six chapters on materials. The processing program, which is the strongest part of the book, begins with a broad overview that serves to broaden the chemist's perspectives and perceptions about the stringent requirements of the electronics industry regarding such, often overlooked, topics as water purity, dopant concentration, nanoscale features, and surface topology. Subsequent chapters, as expected, deal with thin film growth issues related to both elemental and compound semiconductors. Continuing to stress chemical issues while maintaining contact with materials science, the subsequent chapters focus on photolithography, deposition of metals, and plasma etching. While each of these topics has a very broad engineering component, the authors have done a masterful job in writing their chapters with an appreciation for the background and experience of student chemists.

The six chapters on materials deal with corrosion, nanoanalysis, dielectrics, interconnects, ceramics, high critical temperature superconductors, and fuel cells. These form a diverse, and interesting, set of stand-alone chapters.

Throughout, the chapters conclude with a limited set of "homework" problems and a short set of references which, to varying degrees, will prove useful to readers.

J. M. White, University of Texas at Austin

JA965573J

S0002-7863(96)05573-4